Cellular automata for modeling protein folding in lattice models

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We used cellular automata (CA) for the modeling of the temporal folding of proteins [1][2]. Unlike the focus of the vast research already done on the direct prediction of the final folded conformations, we model the temporal and dynamic folding process. The CA model defines how the amino acids interact through time to obtain a folded conformation. We employed the HP model to represent the protein conformations in a lattice, we extended the classical CA models using artificial neural networks for their implementation, and we used evolutionary computing to automatically obtain the models by means of Differential Evolution. Moreover, the modeling of the folding provides the final protein conformation, so we can compare the results with those from direct prediction methods of the final protein conformation.

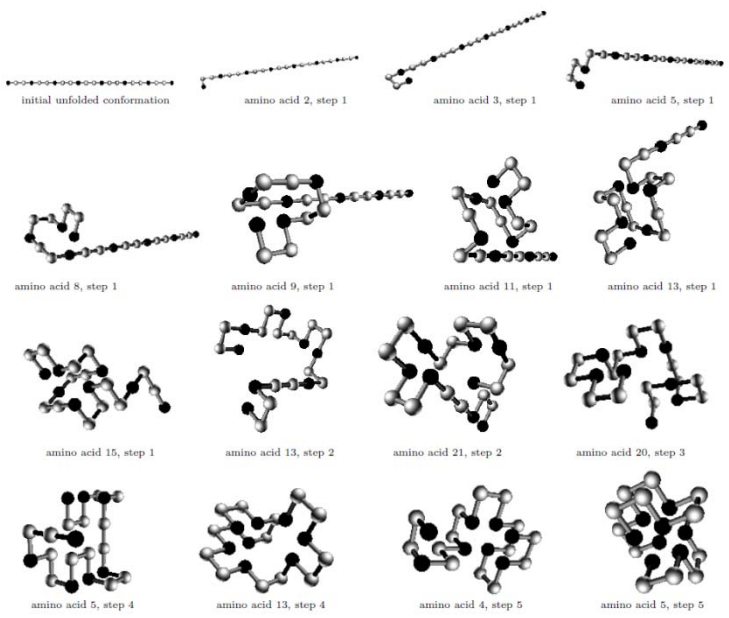

Figure: Example of different temporal steps in the folding process with protein sequence HPPHPPHPPHPPHPPHPPHPPH.

References

[1] Santos, J., Villot, P., Diéguez, M. (2013), "Cellular automata for modeling protein folding using the HP model", *Proc. IEEE Congress on Evolutionary Comp. - IEEE-CEC 2013*, 1586-1593.

[2] Santos, J., Villot, P., Diéguez, M. (2013), "Protein folding with cellular automata in the 3D HP model", *Proc. Intern. Workshop Evolutionary Comp. in Bioinformatics - Genetic and Evol. Comp. Conf. (GECCO 2013)*, 1595-1602.